Goodness of fit tests for weighted histograms

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Abstract

Weighted histogram in Monte-Carlo simulations is often used for the estimation of a probability density function. It is obtained as a result of random experiment with random events that have weights. In this paper the bin contents of weighted histogram are considered as a sum of random variables with random number of terms. Goodness of fit tests for weighted histograms and for weighted histograms with unknown normalization are proposed. Sizes and powers of the tests are investigated numerically.

Key words: chi-square test generalization, multinomial distribution, Monte-Carlo simulation, probability density function estimator, test size
PACS: 02.50.-r, 02.50.Cw, 02.50.Le, 02.50.Ng

1 Introduction

A histogram with m bins for a given probability density function $p(x)$ is used to estimate the probabilities

$$p_i = \int_{S_i} p(x)dx, \ i = 1, \ldots, m \tag{1}$$

that a random event belongs to bin i. Integration in (1) is done over the bin S_i.

A histogram can be obtained as a result of a random experiment with probability density function $p(x)$. Let us denote the number of random events belonging to the ith bin of the histogram as n_i. The total number of events

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in the histogram is equal to $n = \sum_{i=1}^{m} n_i$. The quantity $\hat{p}_i = n_i/n$ is an estimator of p_i with expectation value $\mathrm{E}\,\hat{p}_i = p_i$. The distribution of the number of events for bins of the histogram is the multinomial distribution [1] and the probability of the random vector $(n_1, \ldots, n_m)$ is given by

$$P(n_1, \ldots, n_m) = \frac{n!}{n_1! n_2! \ldots n_m!}\, p_1^{n_1} \ldots p_m^{n_m}, \quad \sum_{i=1}^{m} p_i = 1. \qquad (2)$$

The problem of goodness of fit is to test the hypothesis

$$H_0 : p_1 = p_{10}, \ldots, p_{m-1} = p_{m-1,0} \text{ vs. } H_a : p_i \neq p_{i0} \text{ for some } i, \qquad (3)$$

where p_{i0} are specified probabilities, and $\sum_{i=1}^{m} p_{i0} = 1$. The test is used in a data analyses for comparison theoretical frequencies np_{i0} with the observed frequencies n_i. This classical problem remains of current practical interest. The test statistic

$$X^2 = \sum_{i=1}^{m} \frac{(n_i - np_{i0})^2}{np_{i0}} \qquad (4)$$

was suggested by Pearson [2]. Pearson showed that the statistic (4) has approximately a χ^2_{m-1} distribution if the hypothesis H_0 is true. Improvements of the chi-square test were proposed in [3–5], also known are the likelihood ratio test [6] and an exact test [7]. Review and comparison of different multinomial goodness-of-fit tests was done in [8], a detailed numerical investigation has been given in [9].

Weighted histograms are often obtained as a result of Monte-Carlo simulations. References [10–12] are examples of research works in high energy physics, statistical mechanics and astrophysics using such histograms. Operations with weighted histograms are realised in contemporary systems for data analysis HBOOK [13], Physics Analysis Workstation(PAW) [14] and ROOT framework [15], developed at CERN (European Organization for Nuclear Research, Geneva, Switzerland).

To define a weighted histogram let us write the probability p_i (1) for a given probability density function $p(x)$ in the form

$$p_i = \int_{S_i} p(x)dx = \int_{S_i} w(x)g(x)dx, \qquad (5)$$

where

$$w(x) = p(x)/g(x) \qquad (6)$$

is the weight function and $g(x)$ is some other probability density function. The function $g(x)$ must be larger than 0 for points x, where $p(x) \neq 0$. Weight $w(x) = 0$ if $p(x) = 0$ [16].

The weighted histogram is obtained as a result of a random experiment with probability density function $g(x)$ and weights of events calculated according

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to (6). Let us denote the total sum of weights of events in the ith bin of the weighted histogram as

$$W_i = \sum_{k=1}^{n_i} w_i(k), \qquad (7)$$

where n_i is the number of events at bin i and $w_i(k)$ is the weight of kth event in the ith bin. The total number of events in the histogram is equal to $n = \sum_{i=1}^{m} n_i$, where m is the number of bins. The quantity $\hat{p}_i = W_i/n$ is the estimator of p_i with expectation value $E\,\hat{p}_i = p_i$. Notice that in the case when $g(x) = p(x)$ the weights of events are equal to 1 and the weighted histogram is the usual histogram. For weighted histograms again the problem of goodness of fit is to test the hypothesis

$$H_0 : p_1 = p_{10}, \ldots, p_{m-1} = p_{m-1,0} \text{ vs. } H_a : p_i \neq p_{i0} \text{ for some } i, \qquad (8)$$

where p_{i0} are specified probabilities, and $\sum_{i=1}^{m} p_{i0} = 1$.

In practice the heuristic "chi-square" test statistic is used for this purpose

$$X_h^2 = \sum_{i=1}^{m} \frac{(W_i - np_{i0})^2}{W_{2i}}, \qquad (9)$$

where

$$W_{2i} = \sum_{k=1}^{n_i} w_i(k)^2. \qquad (10)$$

It is expected that if hypothesis H_0 is true then statistic X_h^2 has χ_{m-1}^2 distribution. The recommended minimal number of events in a bin is equal to 25 for application this test [13–15].

The next section of this paper proposes a generalization of the chi-square test for weighted histograms, a goodness of fit test for weighted histograms with unknown normalization is proposed in section 3. To evaluate the tests, in section 4 the sizes and powers of the tests are calculated for numerical examples with different numbers of events, bins and weight functions. The size of the test is compared with the calculated size of the heuristic chi-square test. The comparison demonstrates the superiority of the proposed generalization of chi-square test over the heuristic chi-square test.

2   The test

The total sum of weights of events in ith bin W_i, $i = 1, \ldots, m$ can be considered as a sum of random variables

$$W_i = \sum_{k=1}^{n_i} w_i(k), \qquad (11)$$

where also the number of events n_i is a random value and the weights $w_i(k), k = 1, ..., n_i$ are independent random variables with the same probability distribution function. The distribution of the number of events for bins of the histogram is the multinomial distribution and the probability of the random vector $(n_1, \ldots, n_m)$ is

$$P(n_1, \ldots, n_m) = \frac{n!}{n_1! n_2! \ldots n_m!} \, g_1^{n_1} \ldots g_m^{n_m}, \ \sum_{i=1}^m g_i = 1, \tag{12}$$

where

$$g_i = \int_{S_i} g(x) dx, \ i = 1, \ldots, m \tag{13}$$

is the probability that a random event belongs to the bin i. Integration in (13) is done over the bin S_i.

Let us denote the expectation values of the weights of events from the ith bin as $\mathrm{E}\, w_i = \mu_i$ and the variances as $\mathrm{Var}\, w_i = \sigma_i^2$. The expectation value of the total sum of weights $W_i, i = 1, \ldots, m$ is [17]:

$$\mathrm{E}\, W_i = \mathrm{E} \sum_{k=1}^{n_i} w_i(k) = \mathrm{E}\, w_i \mathrm{E}\, n_i = n \mu_i g_i. \tag{14}$$

The diagonal elements γ_{ii} of the covariance matrix of the vector $(W_1, \ldots, W_m)$ are equal to [17]

$$\gamma_{ii} = \sigma_i^2 g_i n + \mu_i^2 g_i (1 - g_i) n = n \alpha_{2i} g_i - n \mu_i^2 g_i^2, \tag{15}$$

where $\alpha_{2i} = \mathrm{E}\, w_i^2$. The non-diagonal elements $\gamma_{ij}, i \neq j$ are equal to:

$$\begin{aligned}
\gamma_{ij} &= \sum_{k=0}^n \sum_{l=0}^n \mathrm{E} \left[\sum_{u=1}^k \sum_{v=1}^l w_i(u) w_j(v) \right] h(k, l) - \mathrm{E}\, W_i \mathrm{E}\, W_j \\
&= \sum_{k=0}^n \sum_{l=0}^n \mathrm{E}\, (w_i w_j) h(k, l) kl - \mu_i n g_i \mu_j n g_j \\
&= \mu_i \mu_j (-g_i g_j n + g_i g_j n^2) - \mu_i n g_i \mu_j n g_j \\
&= -n \mu_i \mu_j g_i g_j,
\end{aligned} \tag{16}$$

where $h(k, l)$ is the probability that k events belong to bin i and l events to bin j.

If hypothesis H_0 is true then

$$\mathrm{E}\, W_i = n \mu_i g_i = n p_{i0}, \ i = 1, \ldots, m \tag{17}$$

and

$$g_i = p_{i0}/\mu_i, \ i = 1, \ldots, m. \tag{18}$$

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We can substitute g_i to (15) which gives

$$\gamma_{ii} = n(\frac{p_{i0}}{r_i} - p_{i0}^2), \tag{19}$$

where $r_i = \mu_i/\alpha_{2i}$. Substituting g_i into (16) gives

$$\gamma_{ij} = -np_{i0}p_{j0}. \tag{20}$$

Notice that for usual histograms the ratio of moments r_i is equal to 1 and the covariance matrix coincides with the covariance matrix of the multinomial distribution.

Let us now introduce the multivariate T^2 Hotelling statistic

$$(\mathbf{W} - n\mathbf{p}_0)'\Gamma_k^{-1}(\mathbf{W} - n\mathbf{p}_0), \tag{21}$$

where
$\mathbf{W} = (W_1, \ldots, W_{k-1}, W_{k+1}, \ldots, W_m)'$, $\mathbf{p}_0 = (p_{10}, \ldots, p_{k-1,0}, p_{k+1,0}, \ldots, p_{m0})'$ and $\Gamma_k = (\gamma_{ij})_{(m-1)\times(m-1)}$ is the covariance matrix for a histogram without bin k. The matrix Γ_k has the form

$$\Gamma_k = \text{diag}\,(n\frac{p_{10}}{r_1}, \ldots, n\frac{p_{k-1,0}}{r_{k-1}}, n\frac{p_{k+1,0}}{r_{k+1}}, \ldots, n\frac{p_{m0}}{r_m}) - n\mathbf{p}_0\mathbf{p}_0', \tag{22}$$

and the Woodbury theorem [18] can be applied to find Γ_k^{-1}. After that the Hotelling statistic can be written as

$$X_k^2 = \sum_{i\neq k} r_i \frac{(W_i - np_{i0})^2}{np_{i0}} + \frac{(\sum_{i\neq k} r_i(W_i - np_{i0}))^2}{n - \sum_{i\neq k} r_i np_{i0}}. \tag{23}$$

and can be transformed to

$$X_k^2 = \frac{1}{n}\sum_{i\neq k} \frac{r_i W_i^2}{p_{i0}} + \frac{1}{n}\frac{(n - \sum_{i\neq k} r_i W_i)^2}{1 - \sum_{i\neq k} r_i p_{i0}} - n \tag{24}$$

that is convenient for numerical calculations. Asymptotically the vector $\mathbf{W}$ has a normal distribution $\mathcal{N}(n\mathbf{p}_0, \Gamma_k^{1/2})$ [19] and therefore the test statistic (23) has χ_{m-1}^2 distribution if hypothesis H_0 is true. Notice that for usual histograms when $r_i = 1$, $i = 1, \ldots, m$ the statistic (23) is Pearson's chi-square statistic. The expectation value of statistic (23) is equal to

$$\text{E}\,X_k^2 = \frac{1}{n}\sum_{i\neq k} \frac{r_i \text{E}\,W_i^2}{p_{i0}} + \frac{1}{n}\frac{n^2 - 2n\sum_{i\neq k} r_i \text{E}\,W_i + \text{E}\,(\sum_{i\neq k} r_i W_i)^2}{1 - \sum_{i\neq k} r_i p_{i0}} - n. \tag{25}$$

According (17) and (19)

$$\text{E}\,W_i^2 = np_{i0}/r_i - np_{i0}^2 + n^2 p_{i0}^2 \tag{26}$$

and

$$E\left(\sum_{i\neq k} r_i W_i\right)^2 = -n\left(\sum_{i\neq k} r_i p_{i0}\right)^2 + n^2\left(\sum_{i\neq k} r_i p_{i0}\right)^2 + n\sum_{i\neq k} r_i p_{i0} \qquad (27)$$

then

$$E\,X_k^2 = m - 1 + (n-1)\sum_{i\neq k} r_i p_{i0} - n$$

$$+ \frac{n - 2n\sum_{i\neq k} r_i p_{i0} - (\sum_{i\neq k} r_i p_{i0})^2 + n(\sum_{i\neq k} r_i p_{i0})^2 + \sum_{i\neq k} r_i p_{i0}}{1 - \sum_{i\neq k} r_i p_{i0}}$$

$$= m - 1$$

$$(28)$$

as for Pearson's test [20].

Let us now replace r_i with the estimate $\hat{r}_i = W_i/W_{2i}$ and denote the estimator of matrix Γ_k as $\hat{\Gamma}_k$. Then for positive definite matrices $\hat{\Gamma}_k$, $k = 1, \ldots, m$ the test statistic is given as

$$\hat{X}_k^2 = \frac{1}{n}\sum_{i\neq k} \frac{\hat{r}_i W_i^2}{p_{i0}} + \frac{1}{n}\frac{(n - \sum_{i\neq k} \hat{r}_i W_i)^2}{1 - \sum_{i\neq k} \hat{r}_i p_{i0}} - n. \qquad (29)$$

Formula (29) for usual histograms does not depend on the choice of the excluded bin, but for weighted histograms there can be a dependence. A test statistic that is invariant to the choice of the excluded bin and at the same time is Pearson's chi square statistics for the usual histograms can be obtained as the median value of (29) with positive definite matrix $\hat{\Gamma}_k$ for a different choice of excluded bin

$$\hat{X}^2 = \text{Med }\{\hat{X}_1^2, \hat{X}_2^2, \ldots, \hat{X}_m^2\}. \qquad (30)$$

Usage of $\hat{X}^2$ to test the hypothesis H_0 with a given significance level is equivalent to making a decision by voting.

Use of the chi-square tests is inappropriate if any expected frequency is below 1 or if the expected frequency is less than 5 in more than 20% of bins [21]. This restriction known for usual chi-square test is quite reasonable for weighted histograms also and helps to avoid cases when matrix $\hat{\Gamma}_k$ is not positive definite.

Notice also that for case $W_i = 0$ the ratio $\hat{r}_i$ is undefined. The average value of this quantity for nearest neighbors bins with non-zero bin content can be used for approximation of undefined $\hat{r}_i$.

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3 The test for histograms with unknown normalization

In practice one is often faced the case that a histogram is defined up to an unknown normalization constant C. Let us denote a bin content of histograms without normalization as $\check{W}_i$, then $W_i = \check{W}_i C$, and the test statistic (24) can be written as

$$X_k^2 = \frac{C}{n} \sum_{i \neq k} \frac{\check{r}_i \check{W}_i^2}{p_{i0}} + \frac{1}{n} \frac{(n - \sum_{i \neq k} \check{r}_i \check{W}_i)^2}{1 - C^{-1} \sum_{i \neq k} \check{r}_i p_{i0}} - n, \tag{31}$$

with $\check{r}_i = C r_i$. An estimator for the constant C can be found by minimization of (31). The normal equation for (31) has the form

$$\sum_{i \neq k} \frac{\check{r}_i \check{W}_i^2}{p_{i0}} - \frac{(n - \sum_{i \neq k} \check{r}_i \check{W}_i)^2}{(C - \sum_{i \neq k} \check{r}_i p_{i0})^2} \sum_{i \neq k} \check{r}_i p_{i0} = 0 \tag{32}$$

with two solutions

$$\hat{C}_k = \sum_{i \neq k} \check{r}_i p_{i0} \pm \sqrt{\frac{\sum_{i \neq k} \check{r}_i p_{i0}}{\sum_{i \neq k} \check{r}_i \check{W}_i^2 / p_{i0}}} \left(n - \sum_{i \neq k} \check{r}_i \check{W}_i\right), \tag{33}$$

where $\hat{C}_k$ is an estimator of C. We choose the solution with the positive sign because it converges to a constant $C = 1$ for the case of a usual histogram, while the solution with negative sign does not. Substituting (33) to the (31) we get the test statistic

$$\check{X}_k^2 = \frac{\hat{C}_k}{n} \sum_{i \neq k} \frac{\check{r}_i \check{W}_i^2}{p_{i0}} + \frac{1}{n} \frac{(n - \sum_{i \neq k} \check{r}_i \check{W}_i)^2}{1 - \hat{C}_k^{-1} \sum_{i \neq k} \check{r}_i p_{i0}} - n \tag{34}$$

that has a χ_{m-2}^2 distribution if hypothesis H_0 is valid. Formula (34) can be also transformed to

$$\check{X}_k^2 = \frac{s^2}{n} + 2s, \tag{35}$$

where

$$s = \sqrt{\sum_{i \neq k} \check{r}_i p_{i0} \sum_{i \neq k} \check{r}_i \check{W}_i^2 / p_{i0}} - \sum_{i \neq k} \check{r}_i \check{W}_i \tag{36}$$

that is convenient for calculations.

The final statistic $\hat{\check{X}}_k^2$ is obtained by replacing $\check{r}_i$ in (35) with the estimate $\hat{\check{r}}_i = \check{W}_i / \check{W}_{2i}$. As in chapter 2, a test statistic that is "invariant" to choice of the excluded bin can be obtained as the median value of (35) for all possible choices of the excluded bin

$$\hat{\check{X}}^2 = \text{Med} \ \{\hat{\check{X}}_1^2, \hat{\check{X}}_2^2, \ldots, \hat{\check{X}}_m^2\}. \tag{37}$$
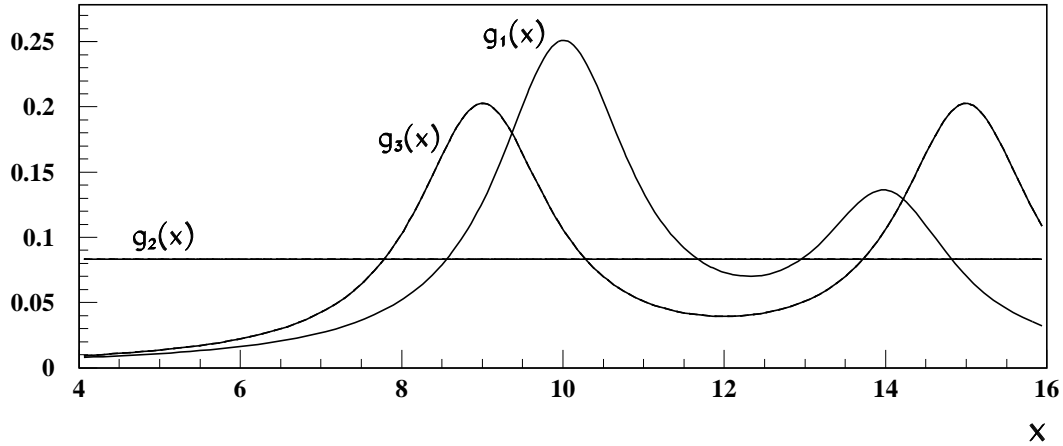
Fig. 1. Probability density functions $g_1(x) = p(x)$, $g_2(x)$ and $g_3(x)$

4 Evaluation of the tests' sizes and power

The tests described herein is now evaluated with a numerical example. We take a distribution

$$p(x) \propto \frac{2}{(x-10)^2 + 1} + \frac{1}{(x-14)^2 + 1} \tag{38}$$

defined on the interval $[4, 16]$ and representing two so-called Breight-Wigner peaks [22]. Three cases of the probability density function $g(x)$ are considered(see Fig.1)

$$g_1(x) = p(x) \tag{39}$$

$$g_2(x) = 1/12 \tag{40}$$

$$g_3(x) \propto \frac{2}{(x-9)^2 + 1} + \frac{2}{(x-15)^2 + 1} \tag{41}$$

Distribution (39) gives an unweighted histogram and the method coincides with Pearson's chi square test. Distribution (40) is a uniform distribution on the interval $[4, 16]$. Distribution (41) has the same form of parametrization as (38), but with different values of the parameters.

Sizes of tests for histograms with different numbers of bins were calculated for nominal values of size equal to $\alpha = 0.05$ and for a nominal value of size equal
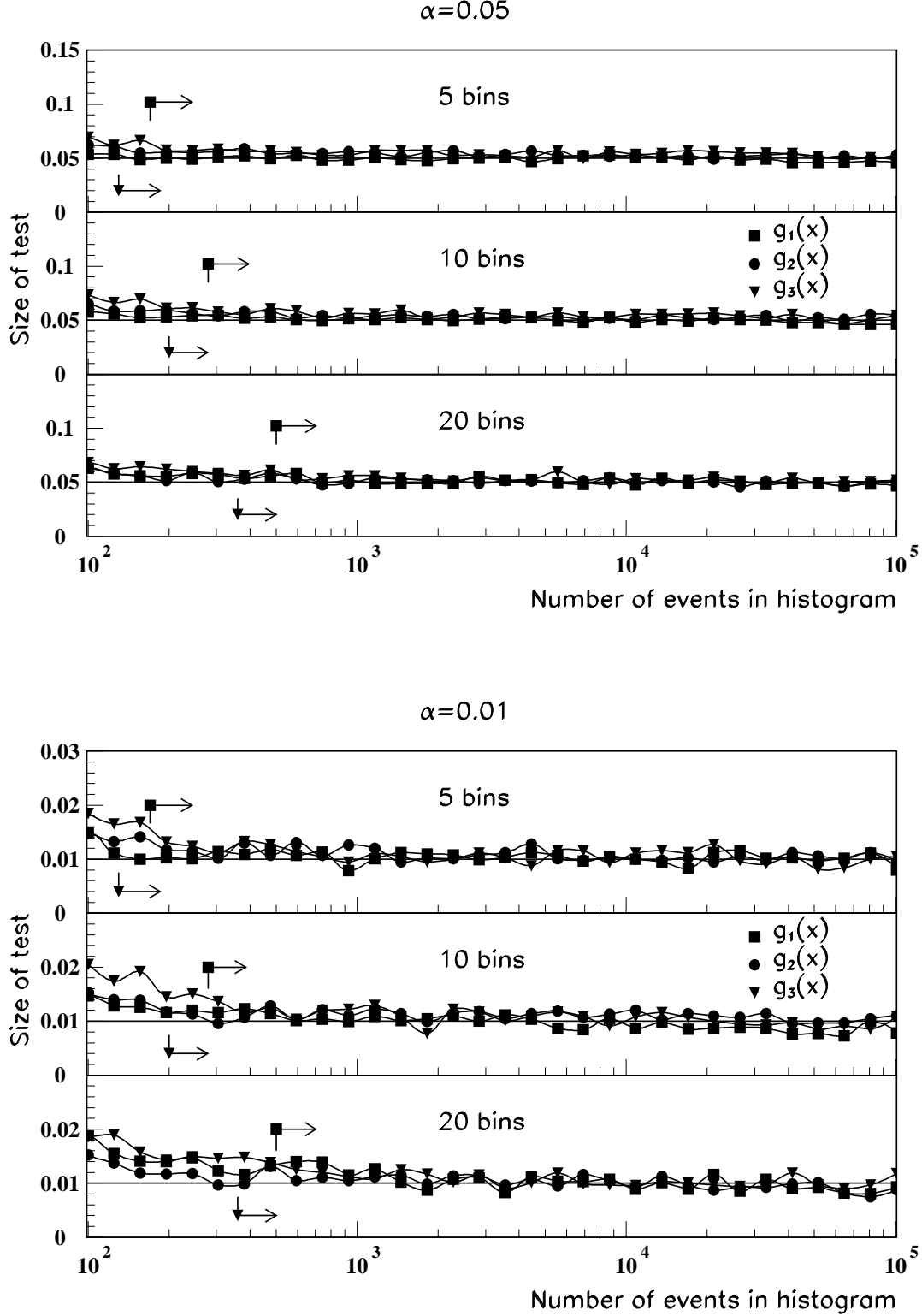
8

$\alpha=0.05$

$\alpha=0.01$

Fig. 2. Sizes of the chi-square tests for histograms with different weight functions and different numbers of bins as a function of the number of events n in the histogram. Arrows show regions with appropriate number of events in histogram for test application.
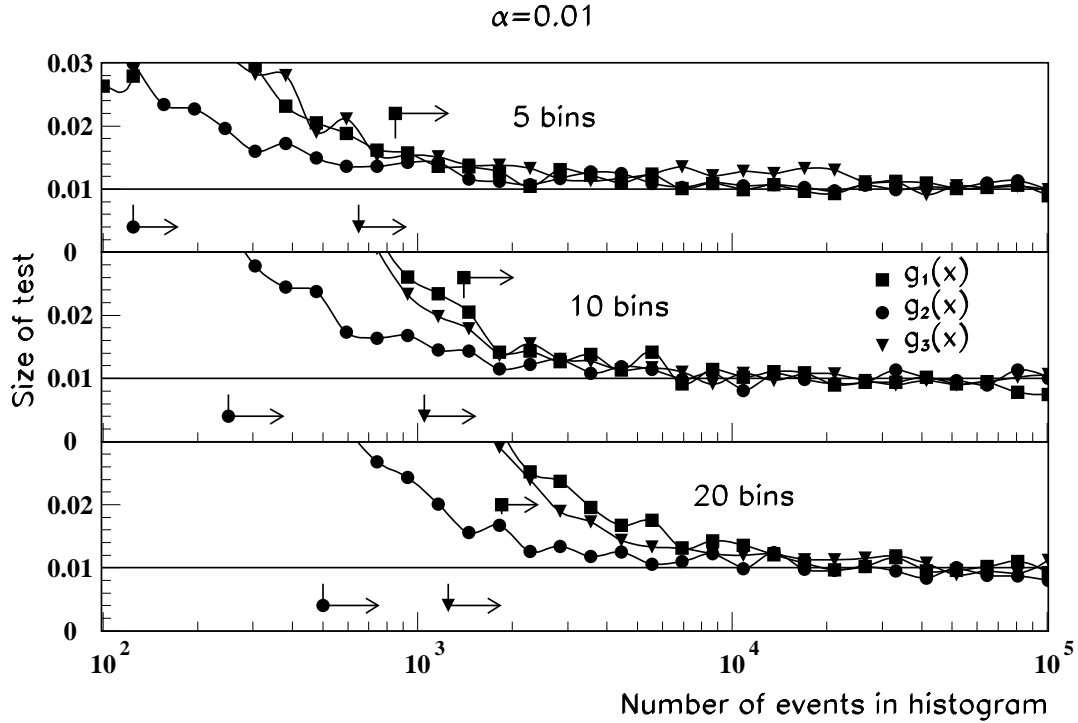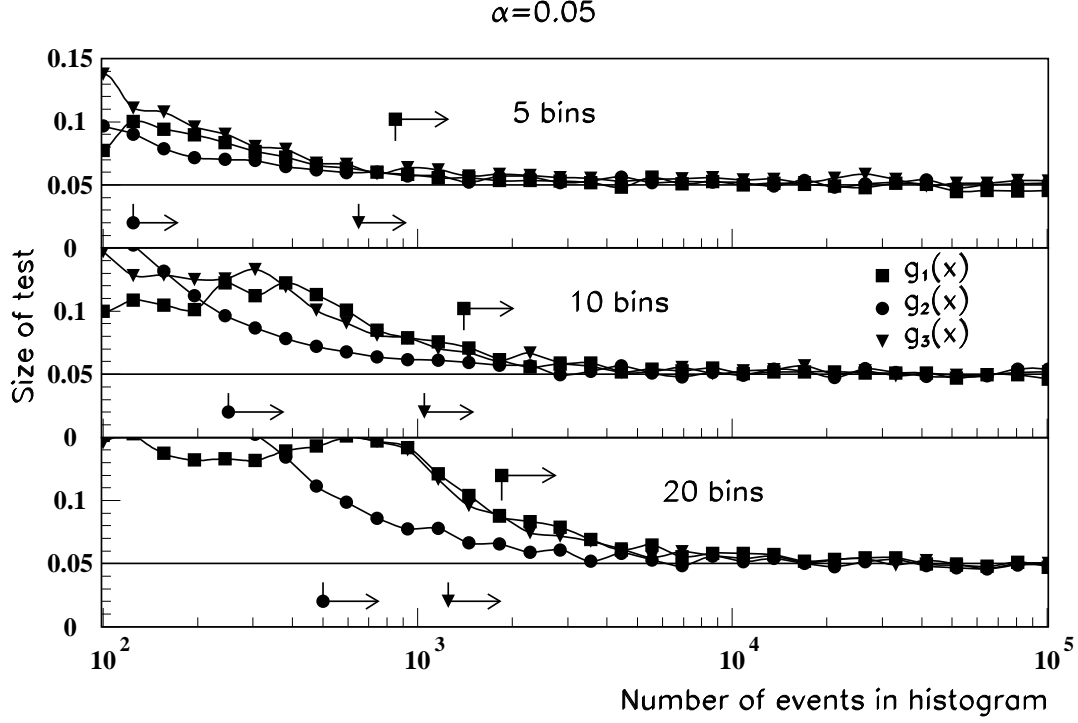
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Fig. 3. Sizes of the heuristic chi-square test for histograms with different weight functions and different numbers of bins as a function of the number of events n in the histogram. Arrows show regions with minimal number of events in bins of histograms equal to 25.
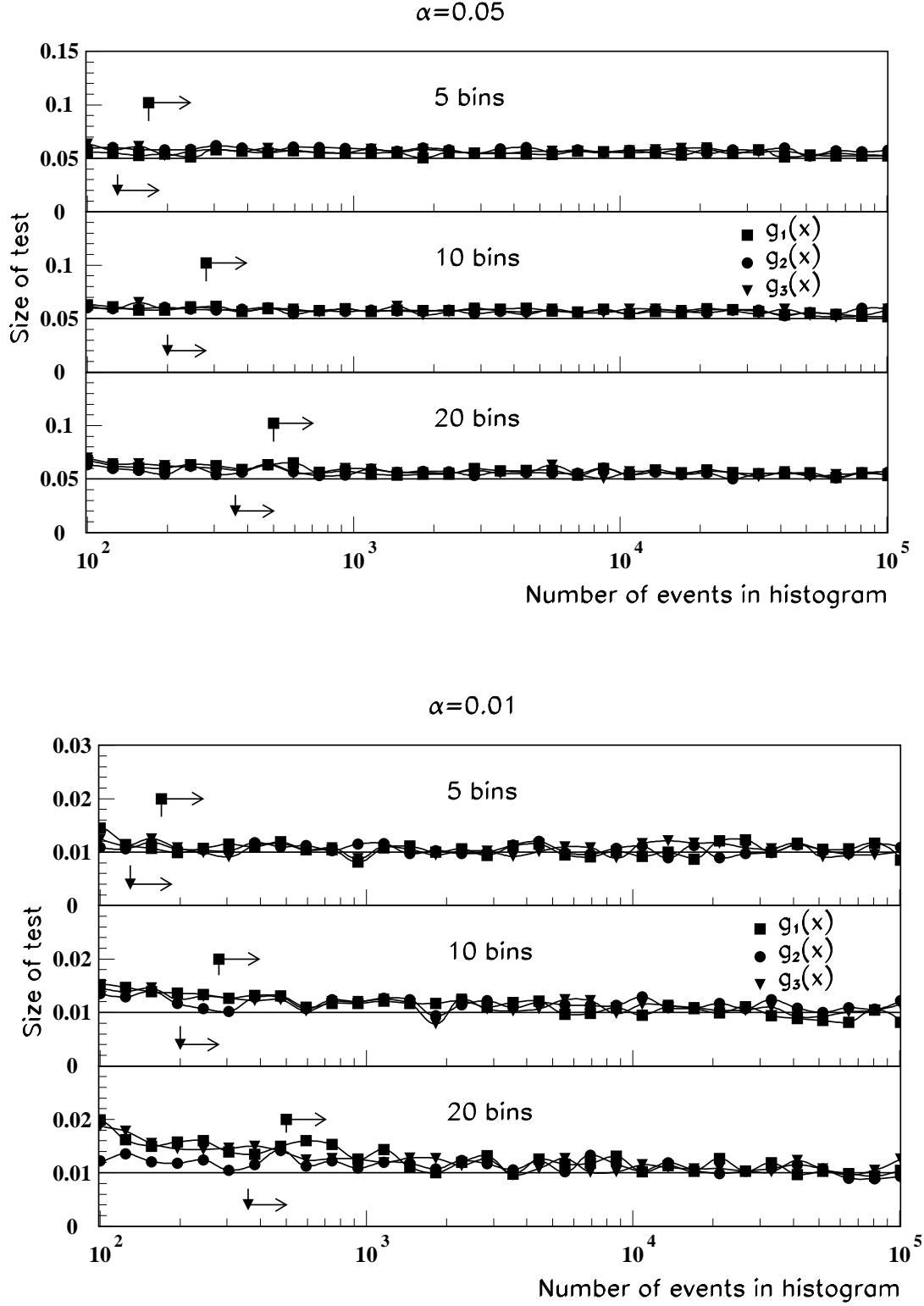
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Fig. 4. Sizes of tests for histograms with unknown normalization for different weight functions and different numbers of bins as a function of the number of events n in the histogram.
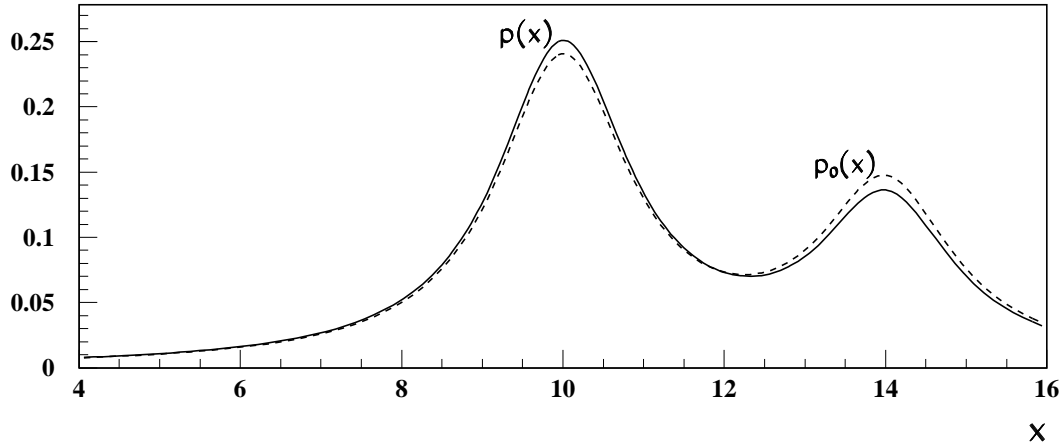
Fig. 5. Probability density function $p(x)$ (solid line) and $p_0(x)$ (dashed line)

to $\alpha = 0.01$ (Fig. 2). Calculations of sizes are done using the Monte-Carlo method based on 10000 runs. It can be noticed that relative deviation of sizes of tests are greater for $\alpha = 0.01$ than for $\alpha = 0.05$. All cases show that test sizes are close to their nominal values for large number n of events in the histogram, and are reasonably close to the nominal values for low statistics of events. The same computation was done for the size of the heuristic test (see Fig. 3). It can be noticed that for large number n of events the sizes of tests tend to the nominal value of the test. For small numbers n of events in the histograms the sizes of the tests are generally greater then the nominal values of tests, although some values of sizes are not shown on the figures because they are too big. Comparison of the two tests bring out clearly the superiority of the generalization of Pearson's test over the heuristic test.

The same study was done for the chi-square test for histograms with unknown normalization. The results of these calculations are presented in Fig. 4. Again all cases show that tests sizes are close to nominal values for large numbers n of events and reasonably close to nominal values for low numbers of events.

The powers of the new chi-square test and the test with unknown normalization were investigated for slightly different values of the amplitude of the second peak of the specified probability distribution function (see Fig. 5):

$$p_0(x) \propto \frac{2}{(x - 10)^2 + 1} + \frac{1.15}{(x - 14)^2 + 1}. \tag{42}$$

The results of these calculations are presented in Fig. 6. Notice that the powers of the tests with unknown normalization are lower than powers of the normalized test. Comparison of the powers of the tests for probability density functions $g_2(x)$ and $g_3(x)$ with powers of the test for function $g_1(x)$ (usual
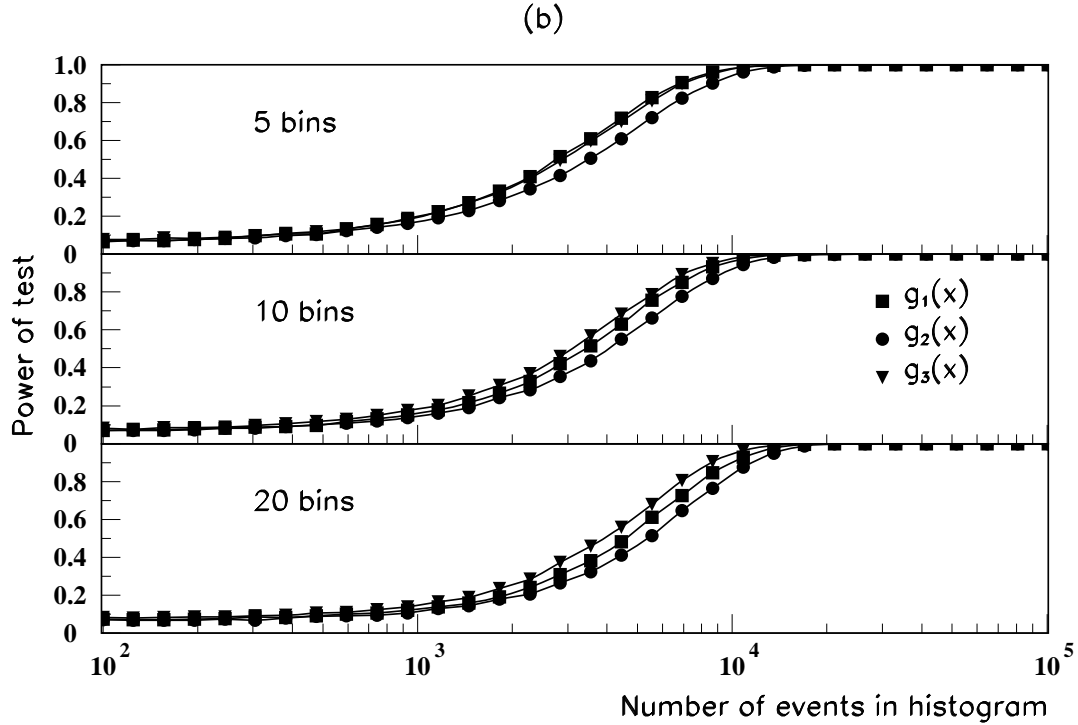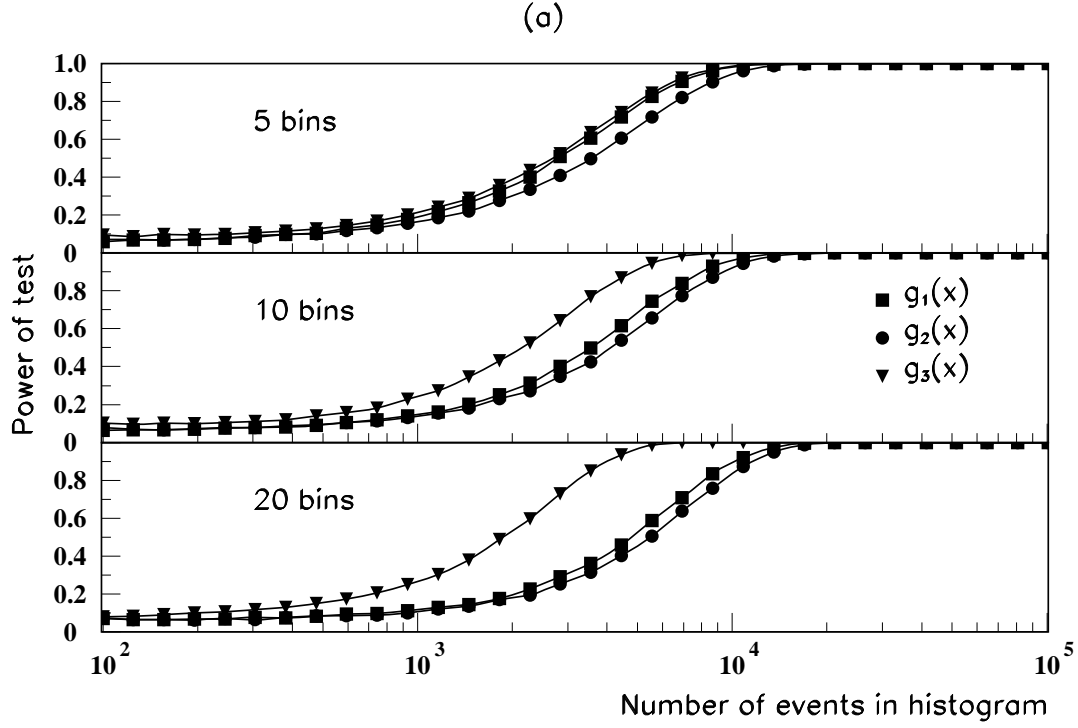
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Fig. 6. Powers of chi-square tests for histograms with different weight functions and different numbers of bins as function of the number of events n in the histogram, (a) chi-square test generalization, (b) chi-square test for histograms with unknown normalization; $\alpha = 0.05$

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unweighted histogram) show that the values of powers are reasonable, as are the sizes of the new tests.

5   Conclusions

A goodness of fit test for weighted histograms is proposed. The test is a generalization of Pearson's chi-square test. Also a goodness of fit test for weighted histograms with unknown normalization is developed. Both tests are very important tools in the application of the Monte-Carlo method as well as in simulation studies of different phenomena. Evaluation of the sizes and powers of those tests was done numerically for histograms with different numbers of bins, different numbers of events and different weight functions. The same investigation was done for the heuristic test used often in practice. Comparison of the results shows the superiority of the new tests compared to the heuristic test.

Acknowledgements

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